PhD position in scientific computing:
Parallel domain decomposition methods for uncertain elliptic PDEs

Level of qualifications required: MS degree or equivalent
Position: PhD student
Gross salary: 2386.29€/month
Starting date: September 2018
Duration: 36 months
Hosting institution: CERFACS, "parallel algorithms" team, Toulouse, France. https://cerfacs.fr/en/parallel-algorithms/
Contact: Paul Mycek (CERFACS), mycek@cerfacs.fr
Keywords: High performance computing, uncertainty quantification, domain decomposition, numerical linear algebra, iterative methods.

Context:
Uncertainty quantification (UQ) is nowadays becoming an integrated component of the numerical simulations, as their fair and complete exploitations require the assessment of the prediction quality. Uncertainty quantification studies often rely on probabilistic approaches, leading to the solution of a stochastic problem, in particular Stochastic Partial Differential Equations (SPDEs). The stochastic problems can be solved by sampling strategies, such as the Monte Carlo method, with thousands or more simulations to be performed to measure variabilities and perform sensitivity analyses. In the case of complex models having high computational cost, direct reuse of existing deterministic solvers may be insufficient to achieve acceptable computational cost and time to solution. Consequently, dedicated solvers exploiting particular structures in the stochastic problem have to be developed.
Recently, a novel domain decomposition approach was proposed for solving elliptic SPDEs [1] [2]. The method is based on a Schur complement approach, where polynomial chaos (PC) surrogates of the boundary-to-boundary maps are constructed in a pre-processing stage. This results in an accelerated Monte Carlo (MC) sampling of the stochastic condensed problem, where samples of the solution at the subdomain boundaries are computed.
The PhD thesis funded by CERFACS will be developed in the framework of a scientific collaboration between Paul Mycek, Olivier Le Maître (LIMSI-CNRS) and Luc Giraud (Inria Bordeaux).

Research work:
The goal of this PhD project is to investigate two ways of making the domain decomposition method more efficient: 1) improve the efficiency and parallel scalability of the sampling stage; and 2) investigate potential dimensionality reduction of the stochastic condensed operator.
The former point will be addressed by looking for appropriate iterative solvers and efficient preconditioners for the linear systems at hand, eventually leading to the development of a high-performance parallel implementation. In particular, asynchronous methods on the one hand, and recycling Krylov methods for multiple right-hand-sides and operators on the other hand, will first be considered. Another potential route for improving the efficiency of the sampling stage is to exploit the *similarity* between realizations through Markov Chain Monte Carlo (MCMC) sampling.
To address the latter point, Karhunen-Loève decomposition or low rank approximation of the condensed (boundary-to-boundary) operator will be investigated. In that context, hierarchical matrices (H-matrices) may be considered.
The successful candidate will be expected to participate in meetings (internal seminars, thematic meetups, conferences, teleconference and in-person meetings with the supervisors and partners), and to participate in the writing of scientific communications (technical reports, scientific journal and conference papers, …).

Required skills:

- Strong background in scientific computing, in particular:
  - numerical methods for partial differential equations,
  - numerical methods for solving linear systems of equations.
- Good programming skills.

Desired skills:

- C++ programming skills.
- Experience in parallel computing using MPI.
- Experience in domain decomposition methods, stochastic computing and/or numerical linear algebra would be a plus.

How to apply: Send a CV and a cover letter to mycek@cerfacs.fr.

References:

[1] A. Contreras, P. Mycek, O. Le Maître, F. Rizzi, B. Debusschere and O. Knio, "Parallel Domain Decomposition Strategies for Stochastic Elliptic Equations. Part A: Local KL Representations," *SIAM Journal on Scientific Computing,* 2018 (in press).

[2] A. Contreras, P. Mycek, O. Le Maître, F. Rizzi, B. Debusschere and O. Knio, "Parallel Domain Decomposition Strategies for Stochastic Elliptic Equations. Part B: Accelerated Monte-Carlo Sampling with Local PC," *SIAM Journal on Scientific Computing,* 2018 (in press).